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COULOMB-BORN ELECTRON IMPACT EXCITATION CROSS-SECTIONS FOR ATMOSPHERIC IONS

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Mission Research Corporation

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20 ABSTRACT (Continue on reverse side if necessary and identify by block number)

Coulomb-Born electron impact excitation cross-sections for thirty ground state transitions of the first three ions of nitrogen and oxygen have been computed for electron energies ranging from the threshold to 300 eV. Effective Gaunt factors for use in estimating cross-sections semi-empirically were also calculated and the reliability of such estimations is discussed. Comparisons with more elaborate theoretical cross-section calculations indicate that the Coulomb-Born

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20. ABSTRACT (Continued).

results appear to over-estimate the cross-section near the threshold for intra-shell transitions ($\Delta n = 0$, where n is the principle quantum number), but not for the inter-shell transitions ($\Delta n \neq 0$).

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SECTION 1

INTRODUCTION

Electron impact excitation cross-sections for ions are required in the study of a wide variety of phenomena. The cross-sections for atmospheric ions are of particular interest. Unfortunately measurements for ions have so far been restricted to simple ions such as He^+, Ca^+, and Ba^+ [1-3]. These ions are either single electron systems or have one electron outside a closed shell. We shall refer to all such systems as "one electron" ions. A few very recent experiments have been done on more complicated species such as Ar^+ [4,5]. However, these experiments have, so far, yielded only excitation functions for certain excited levels. Extracting absolute cross-sections from such data requires a knowledge of cascading effects, among other things. The only atmospheric ion for which an experimental cross-section is available is the molecular species, N_2^+ [6]. Experimental excitation rate constants for highly stripped ions such as NIV, NV, OV, OVI, and OVII have, however, been reported and are reviewed in Reference 7.

Theoretically, the situation is only slightly better. Until recently, ab initio calculations were restricted almost exclusively to one electrons ions. Estimates of excitation cross-sections for atmospheric ions were usually obtained via the Bethe´-Seaton formula[8]. Such cross-sections are essentially semi-empirical since they require the knowledge of an "effective Gaunt factor", $\bar{g}$. Although this $\bar{g}$ parameter can, in principle, be computed theoretically, in practice the values used are taken from tabulations of Allen[9]. Allen's listed values are, themselves, estimates based on early

Coulomb-Born calculations for one electron systems[10]. Many applications require cross-sections for a large number of excitations and the Bethe'-Seaton formula is ideally suited to such calculations from the standpoint of convenience if not accuracy.

Ab initio methods range from the Coulomb-Born (CB-I) approximation, which is the simplest, to the multi-configuration close-coupling (CC) approach which, as its name implies, attempts to include the effects of configuration interaction as well as the mutual interaction effects of the colliding election and the ion potential.

Last year we reported on a CB-I calculation for the resonance transition of NII[11]. This year we have extended the work to cover a number of the allowed ground configuration excitations of the first three ions of nitrogen and oxygen. A correction is made to the previously reported NII cross-section and a comparison with the few other computations available is made. A brief discussion of the validity of Allen's $\bar{g}$ values is also presented. The lack of experimental data, however, makes it rather difficult to assess the accuracy of the theoretical results. As will be seen, the CB-I values are generally higher than the presumably more accurate CC results. This can be attributed to a variety of error sources in the CB-I approach. Estimating the direction of error introduced by CB-I or any other quantum mechanical approximation is much more difficult. Indeed, the error direction may be different from ion to ion and from transition to transition within a given ion. This kind of situation is similar to that found for the calculation of oscillator strengths, wherein certain transitions are very sensitive to particular form of the approximate wave function used to do the calculation. It seems likely that an analogous situation may occur for cross-section determinations since the matrix elements involved are somewhat similar.

SECTION 2

COULOMB-BORN APPROXIMATION

A detailed discussion of the theoretical derivation of the CB-I method is contained in Reference 11. We shall only briefly review the basic formula used here. The cross-section, σ, with consistent neglect of spin and exchange effects, is written

$$\sigma(n_0L_0\text{-}nL) = \frac{\pi a_0^2}{\omega_{L_0} k_0^2} \Omega(n_0L_0 - nL) \qquad (1)$$

where $\Omega(n_0L_0 - nL)$ is the collision strength for the ion transition from the state n_0L_0 to the state nL, k_0^2 is the incident electron energy in Rydbergs and ω_{L_0} is the statistical weight of the initial state and with neglect of spin is given by $(2L_0+1)$. Since the CB-I approximation neglects exchange, the spin contribution to σ can be factored out and the collision strength, which is independent of spin, is given by

$$\Omega(n_0L_0\text{-}nL) = \sum_{L^T,\ell_0,\ell} (2L^T+1)\left|-2i\ R(nL\ell,\ n_0L_0\ell_0|L^T)\right|^2 \qquad (2)$$

Here L^T is the total angular momentum of the atomic plus incident electron system, and ℓ_0 and ℓ are the initial and final incident electron angular momentum values. The reactance matrix, R is defined by

$$R(nL\ell, n_0L_0\ell_0|L^T) = 2\sum_{\lambda} f_\lambda(L\ell, L_0\ell_0|L^T)\alpha_\lambda(L, L_0)\ z_\lambda(k_0\ell_0, n_0\tilde{\ell}_0|k\ell, n\tilde{\ell}) \qquad (3)$$

The $f_\lambda(L_0\ell_0, L\ell|L^T)$ are coefficients tabulated by Percival and Seaton[12], and the $\alpha_\lambda(L_0, L)$ factor is required for transitions involving equivalent electrons. For one electron type excitations $\alpha_\lambda(L_0, L)$ is unity and Equation (3) reduces to the well-known CB-I equations of Von-Regemorter[13] for one electron system. The $z_\lambda(k_0\ell_0, n_0\tilde{\ell}_0|k\ell, n\tilde{\ell})$ functions are essentially the matrix elements of the initial and final electron partial wave functions over the atomic potential as detailed in Reference 11. The $\tilde{\ell}_0$ and $\tilde{\ell}$ are the corresponding initial and final angular momentum values of the atomic orbitals undergoing the excitation.

The angular momentum coupling scheme contained in Equation (3) imposes certain restrictions on the values of λ, ℓ and ℓ_0 that will give non-zero contributions to the R-matrix. Additionally, since the vector coupling scheme requires both $(\lambda+L+L_0)$ and $(\lambda+\tilde{\ell}+\tilde{\ell}_0)$ to be even, it can be seen that for s - p transitions ($\Delta\tilde{\ell} = \pm 1$) only the $\lambda = 1$ term contributes, and hence ΔL is restricted to odd values. This means that the optically allowed $\Delta L = 0$ transitions are predicted to have zero cross-sections in the CB-I approximation. A similar result was found by Sharpton, et al.[14] in their Born calculations on neon electron impact excitation cross-sections. They also report experimental data which suggest that the measured values for the cross-sections, which the Born method predicts to be zero, generally tend to be smaller than the cross-sections which are predicted to be non-zero.

The evaluation of the $\alpha_\lambda(L, L_0)$ factors has been described in Reference 11. Part of this procedure has now been programmed for the computer. The program requires as input, the appropriate L-S eigenfunctions for the initial and final atomic states. This computer code was checked by evaluating $\alpha_\lambda(L, L_0)$ factors for transitions involving complementary configurations. For example the transitions, $(s^2p^2\text{-}sp^3)$ and $(s^2p^3\text{-}p^2s)$, should

give identical α_λ values. Additionally the program correctly computes α_λ values of unity for one-electron transitions. As a result of this checking procedure an error was discovered in the previously hand calculated value $\alpha_\lambda(L_0, L)$ for the NII $[2s^2\ 2p^2(^3P) - 2s2p^3(^3D)]$ excitation, due to an error in the sign of the L-S eigenfunction of the ^3P term. Ideally, the determination of the L-S eigenfunctions should also be automated[15]. For the present work, however, these functions were evaluated by hand using two different but equivalent procedures in an effort to insure their correctness. Table 1 in the next section gives the numerical values of the $\alpha_\lambda(L_0, L)$ values used here.

Finally we note that in the evaluation of the R-matrix in Equation (3) we have used Cowens[16] HX atomic radial functions as previously described in Reference 11. The transition energies were taken from Moore[17].

SECTION 3

RESULTS AND DISCUSSION

In Table 1, we list the transitions for which CB-I cross-sections have been computed. The results are displayed graphically in Figures 1 - 6. Before entering into a detailed discussion of the results, we note here that the corrected CB-I cross-section for the NII ^3P-^3D resonance transition is 2½ times larger than the previously reported value[11]. Thus certain parts of the discussion contained in Section 4 of Reference 11 are invalid. The corrected cross-section is now in better agreement at intermediate energies with the only other theoretical calculation available[18] and it is internally consistent with all of the other CB-I values obtained here, as well as with the results of other workers which have been obtained in the past year.

The variation in magnitude of the different cross-sections for a given ion can be fairly large. However, a few trends are immediately apparent from Figures 1 - 6. Perhaps the most notable feature is that the cross-sections for intra-shell transitions (transitions involving orbitals with the same principal quantum number, n) are generally larger than the cross-sections for intershell transitions ($\Delta n > 0$). This trend agrees with the CC result of Ormande, et al.[18] For the NIV $2s^2$-2snp (^1S-^1P) transitions with n = 2 and 3. Tully[19] has computed CB-I collision strengths for the (1^1S-n^1P) series of helium-like ions with atomic numbers, Z = 3, 4, and 8. For a given Z value and incident electron energy in threshold units, his collision strengths decrease with increasing n. The helium-like transitions are

Table 1. Atmospheric Ion Transitions for Electron Impact Excitation Cross-Sections.

Species	Transition Configuration	Terms	α_λ^2	Energy (eV)
NII	$2s^22p^2 - 2s2p^3$	$^3P - {}^3D$	5/6	11.44
		$^3P - {}^3S$	4/3	19.23
		$^1D - {}^1P$	5/6	18.78
		$^1S - {}^1P$	4/3	16.62
	$2p^2 - 2p3s$	$^1D - {}^1P$	5/3	16.60
		$^1S - {}^1P$	2/3	14.44
	$2p^2 - 2p3d$	$^1S - {}^1P$	4/3	19.57
NIII	$2s^22p - 2s2p^2$	$^2P - {}^2D$	5/6	12.53
		$^2P - {}^2S$	1/3	16.24
	$2p - 3s$	$^2P - {}^2S$	1	27.44
	$2p - 3d$	$^2P - {}^2D$	1	33.13
NIV	$2s^2 - 2s2p$	$^1S - {}^1P$	2	16.20
	$2s^2 - 2s3p$	$^1S - {}^1P$	2	50.16
OII	$2s^22p^3 - 2s2p^4$	$^4S - {}^4P$	1	14.87
		$^2P - {}^2D$	5/12	15.56
		$^2P - {}^2S$	2/3	19.25
	$2p^3 - 2p^23s$	$^4S - {}^4P$	1	22.99
		$^2P - {}^2D$	5/12	20.64
		$^2D - {}^2P$	5/4	20.11
OIII	$2s^22p^2 - 2s2p^3$	$^3P - {}^3D$	5/6	14.86
		$^3P - {}^3S$	4/3	24.41
		$^1D - {}^1P$	5/6	23.58
		$^1S - {}^1P$	4/3	20.74
	$2p^2 - 2p3s$	$^1D - {}^1P$	5/3	31.34
		$^1S - {}^1P$	2/3	28.50
	$2p^2 - 2p3d$	$^1S - {}^1P$	4/3	35.90
OIV	$2s^2 2p - 2s2p^2$	$^2P - {}^2D$	5/6	15.71
		$^2P - {}^2S$	1/3	20.35
	$2p - 3s$	$^2P - {}^2S$	1	44.31
	$2p - 3d$	$^2P - {}^2D$	1	51.98

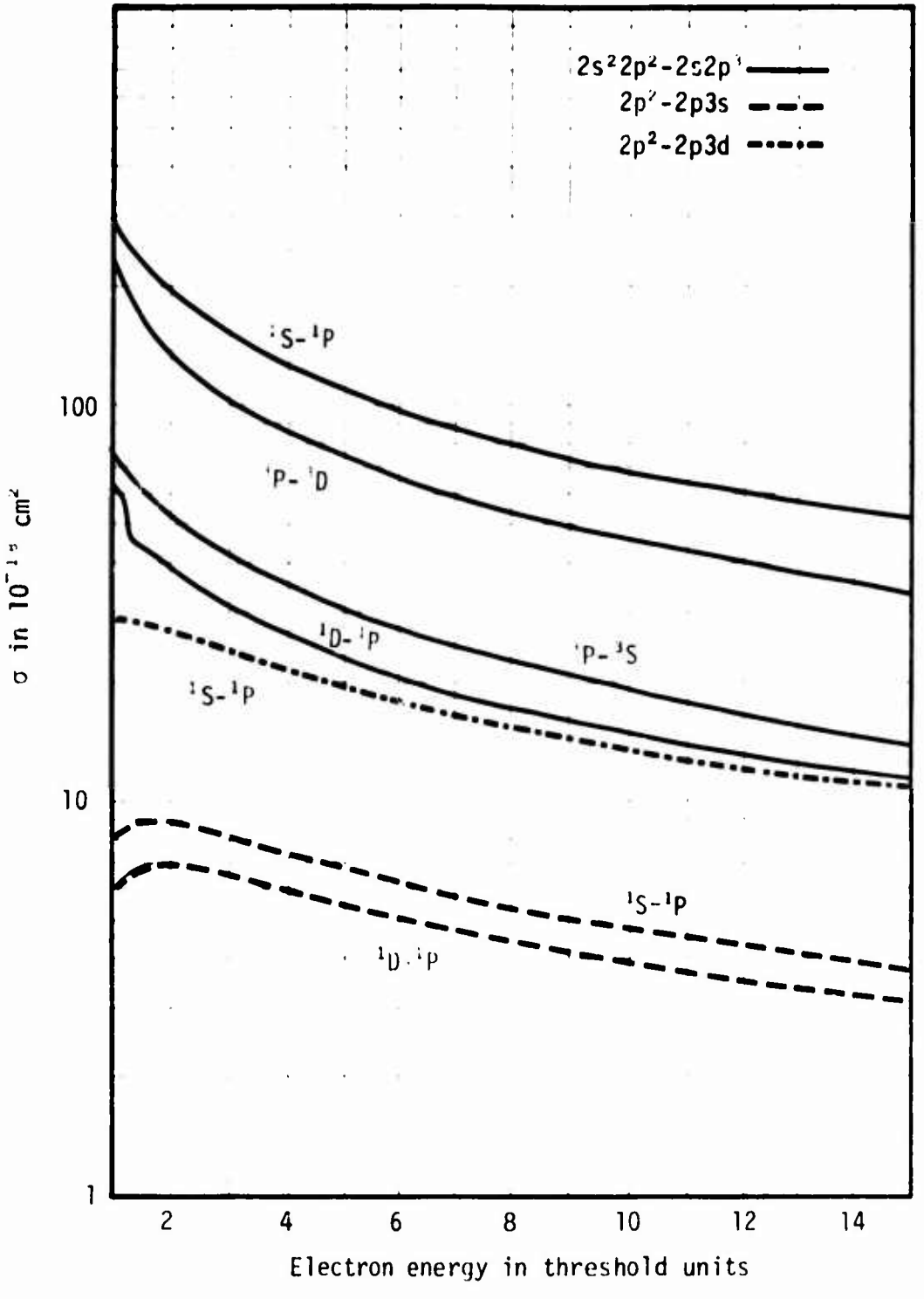

Figure 1. NII Coulomb-Born cross-sections for electron impact excitation.

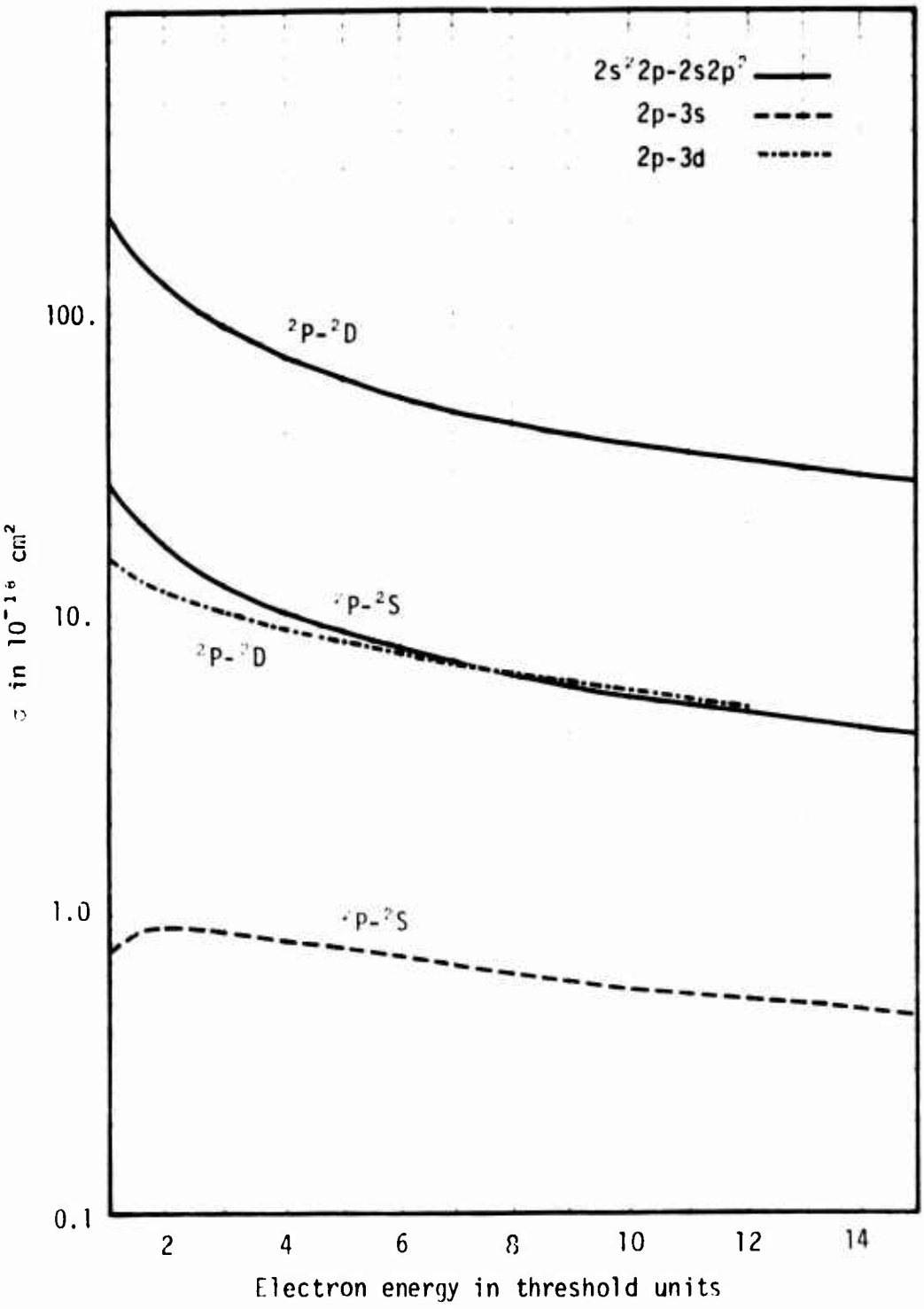

Figure 2. NIII Coulomb-Born cross-sections for electron impact excitation.

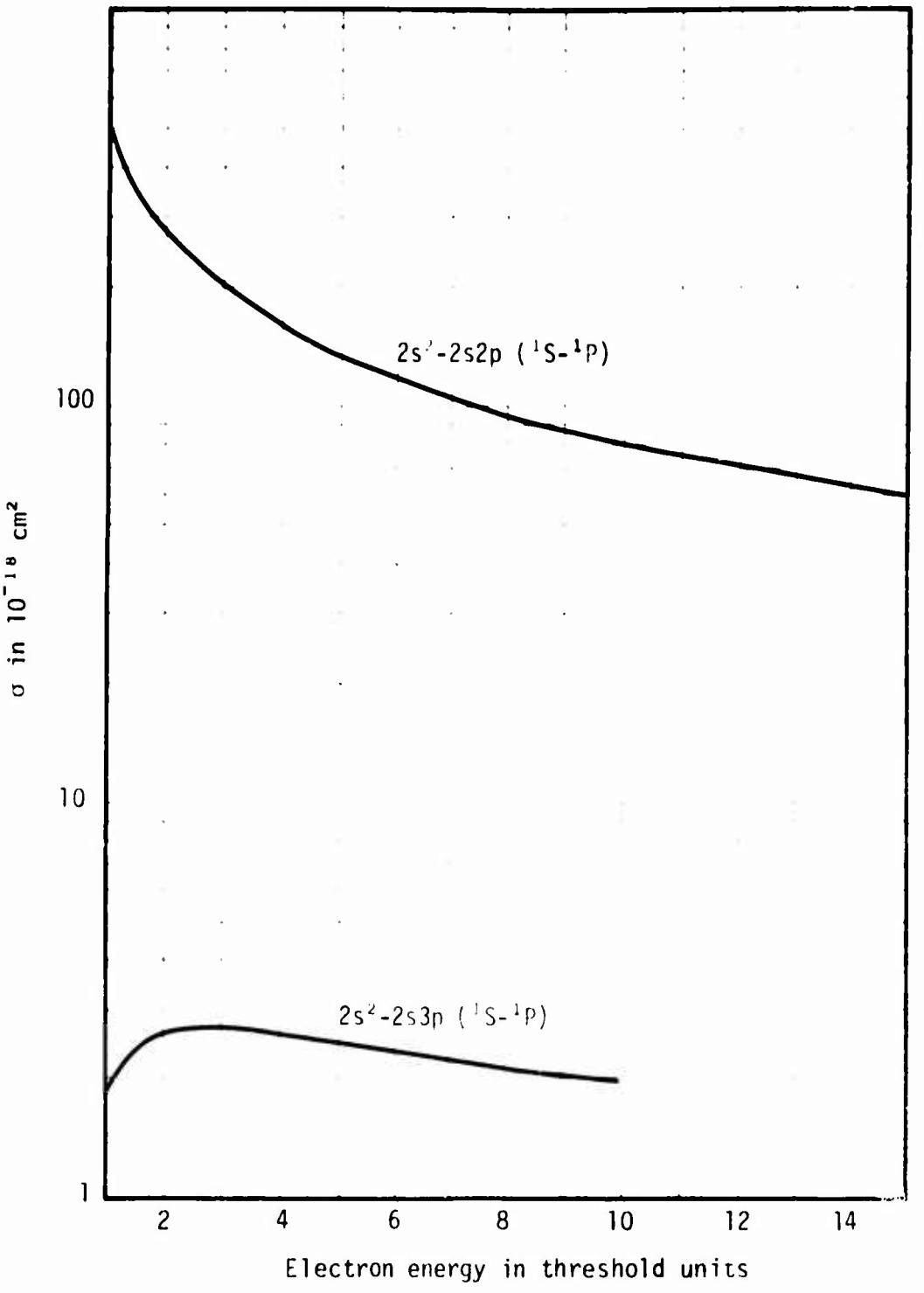

Figure 3. NIV Coulomb-Born cross sections for electron impact excitation.

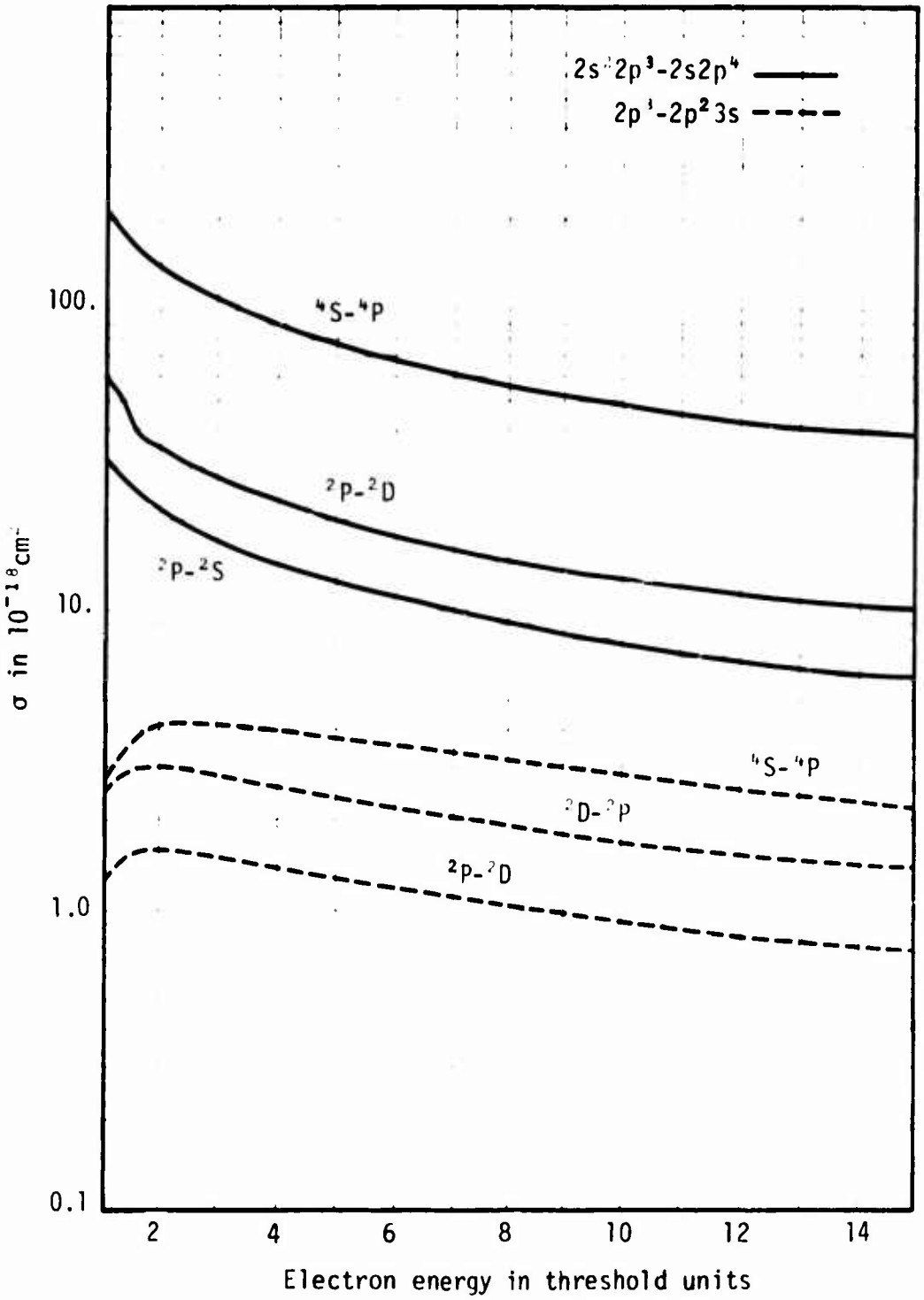

Figure 4. OII Coulomb-Born cross-sections for electron impact excitation.

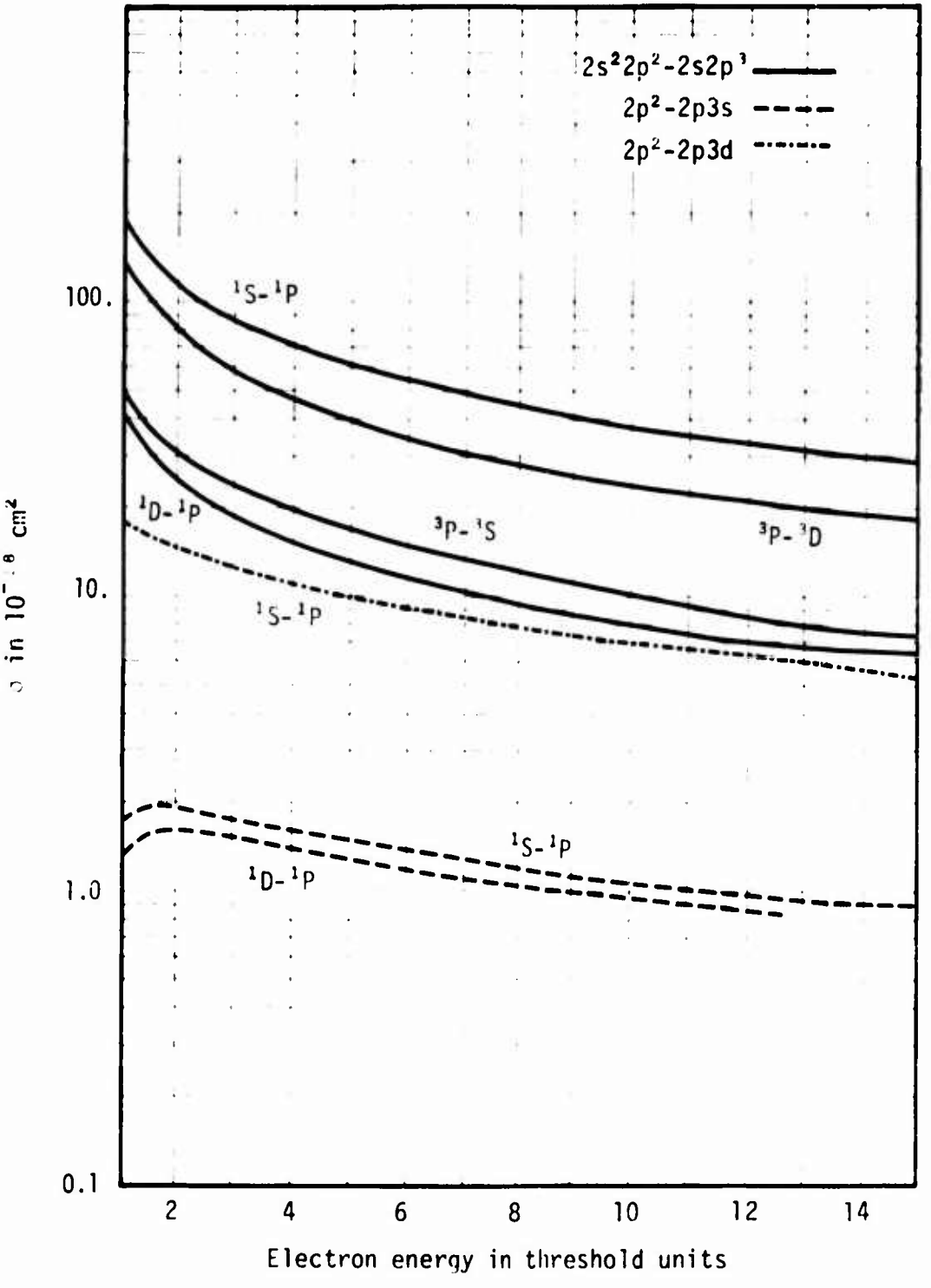

Figure 5. OIII Coulomb-Born cross-sections for electron impact excitation

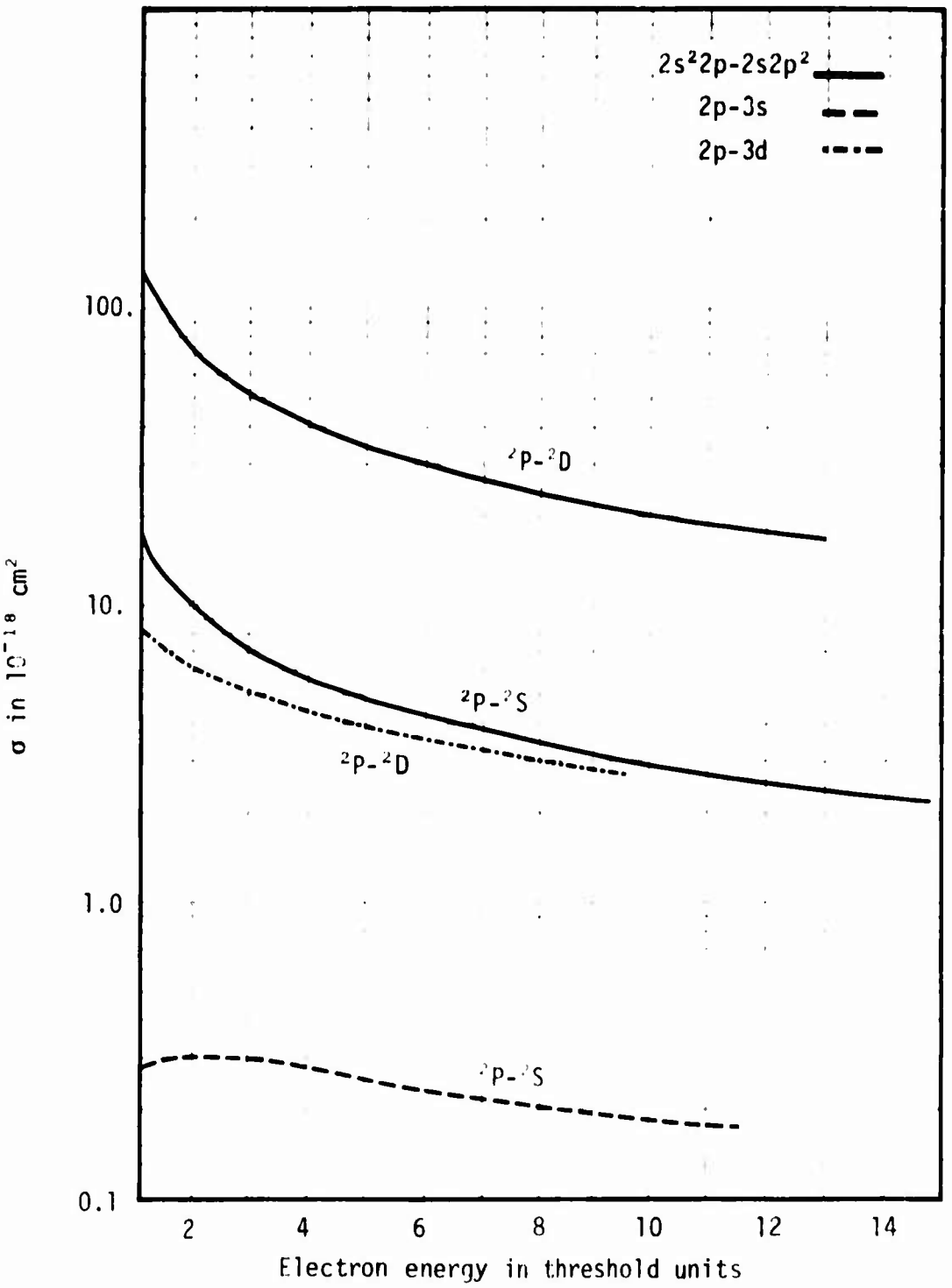

Figure 6. OIV Coulomb-Born cross-sections for electron impact excitation.

perhaps most comparable to the NIV system as both excitations are of the type, ns^2-$nsn'p$. The hydrogen-like ion cross-sections of Tully[20] also exhibit this same behavior. These are all relatively simple systems for which the transition energy is also increasing with Δn. This is not the case for the NII and OIII ions reported on here, so the trend cannot be accounted for solely as a function of increasing transition energy.

A second trend that can be observed is that for a given transition, the cross-section for atomic number Z=8 (oxygen) is smaller than the corresponding transition for Z=7 (nitrogen). This is also in agreement with Tully's[19] results for the helium-like (1^1S-n^1P) series. Osterbrooks[21] computed collision strengths in the CC approximation for the $2s^2$-2s2p (^1S-^1P) transition of the iso-electronic series BII, CIII, NIV, OV, and Ne VII exhibit a similar trend. As Z increases in an iso-electronic series, the atomic electrons are more tightly held to the central nucleus and it becomes more difficult to excite them.

COMPARISONS WITH OTHER AB INITIO CALCULATIONS

Figures 7 - 12 compare the CB-I cross-sections computed here with the multi-configuration CC results reported by Ormande, et al.[18] In every case, except for the excellent agreement of the inter-shell 2s-2p NIV excitation, the CB-I values are larger than the presumably more accurate CC values, particularly near the threshold. However, the intra-shell CB-I cross-sections fall off rather rapidly between one and three threshold units and in most cases the two methods appear to be converging satisfactorily at higher energies as they should. The one exception to this statement is the OII resonance excitation and here the CC curve does not extend out far enough to draw any conclusions as to its eventual high energy behavior.

In general, the agreement between CC and CB-I results improve with increasing charge. As the charge on an ion increases, the long-range coulombic forces between the colliding electron and the ion become more important and the CB-I method which neglects short-range interactions, becomes a much better approximation to the true physical situation.

In the absence of experimental data, it is tempting to use the CC results in their stead. Ormande, et al.[18] estimate that their cross-sections for neutral nitrogen and oxygen have an accuracy of about 5% and they expect that their ion values have a similar accuracy, except for their OII result for which they report an error limit of 25% or less based on convergance considerations. The problem of convergance in the CC method has been addressed by several other workers and is still subject to considerable controversy. Seraph and Seaton[22] have compared their CC calculations with Ormande's[18] results for the forbidden NII transitions among the ground configuration terms and they find that inclusion of the higher configurations did not give a large change in the computed cross-sections near the threshold. This is in disagreement with the Ormande's results. The conflict is significant for predicting resonance peaks, but is somewhat less so with respect to cross-section at higher energies. Seraph and Seaton place a 10% error limit on their results and we can infer from this that the ion CC results of Ormande are perhaps no better than this.

At the threshold our CB-I cross-sections differ from Ormande's by a factor of 6 for OII and by factors of from 1.5 to 2.0 for all the other transitions for which comparisons can be made. For energies greater than two threshold units the differences are in the 15% to 35% range except for the OII cross-section which still differs by a factor of 2.5 at two threshold units.

There are a few other calculations available on simpler ion systems for which comparisons between CB-I and CC results have been made. The

results for He^+ for which exact wavefunctions are available have been summarized by Moiserwitsch and Smith[23] and the CC cross-sections are generally lower than the corresponding CB-I values. For neutrals, however, the trend is not so clear. The CB-I method does not allow for distortion of the colliding electron wavefunction. A scheme which does allow for this is called the Distorted Wave (DW) method. Flowers[24] has compared his DW calculations with both CB-I and some CC results for NV. For most of the transitions considered both the DW and CC results are smaller than the corresponding CB-I values. Such results are strictly comparable only when the same atomic wavefunctions are used throughout. Flower's DW calculations employed Configuration Interaction (CI) wavefunctions while the CC results did not. Thus the effect of including distortion in the calculation cannot be separated from the effect of including CI. Another source of error in the CB-I approach is the neglect of exchange. At present there is no simple or reliable way of estimating the effects of the various possible approximations[7] for the type of transitions under consideration here and the theoretical data available is too limited to warrant any definite conclusions. The available theoretical evidence suggests that the CB-I method will tend to over-estimate the cross-section near the threshold for intra-shell transitons, but that it can give satisfactory results at intermediate and higher energies where the computational labor involved in the CC scheme becomes prohibative.

COMPARISONS WITH THE SEMI-EMPIRICAL ESTIMATES

Figures 7 - 12 also show the semi-empirical cross-sections that are obtained by using the Bethe'-Seaton formula[8]. Allen's[9] $\bar{g}$ values are used and the oscillator strengths are taken from the NBS tabulations of Weise, et al.[25] For the intra-shell cross-sections, the semi-empirical values are below both the CC and the CB-I results by sometimes rather large amounts, except for OII. This transition, however, appears to give somewhat

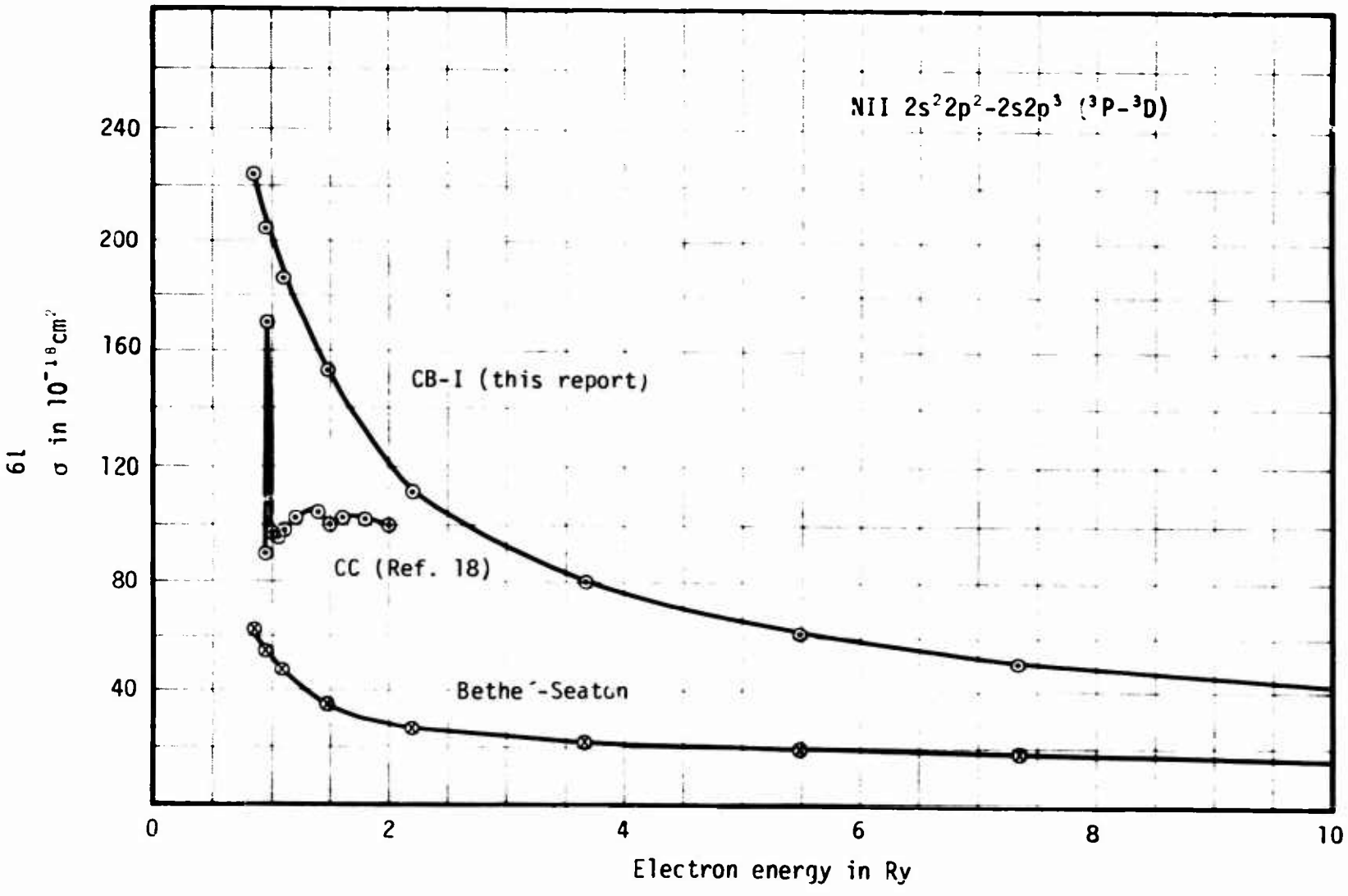

Figure 7. Comparison of theoretical electron impact excitation cross section for NII.

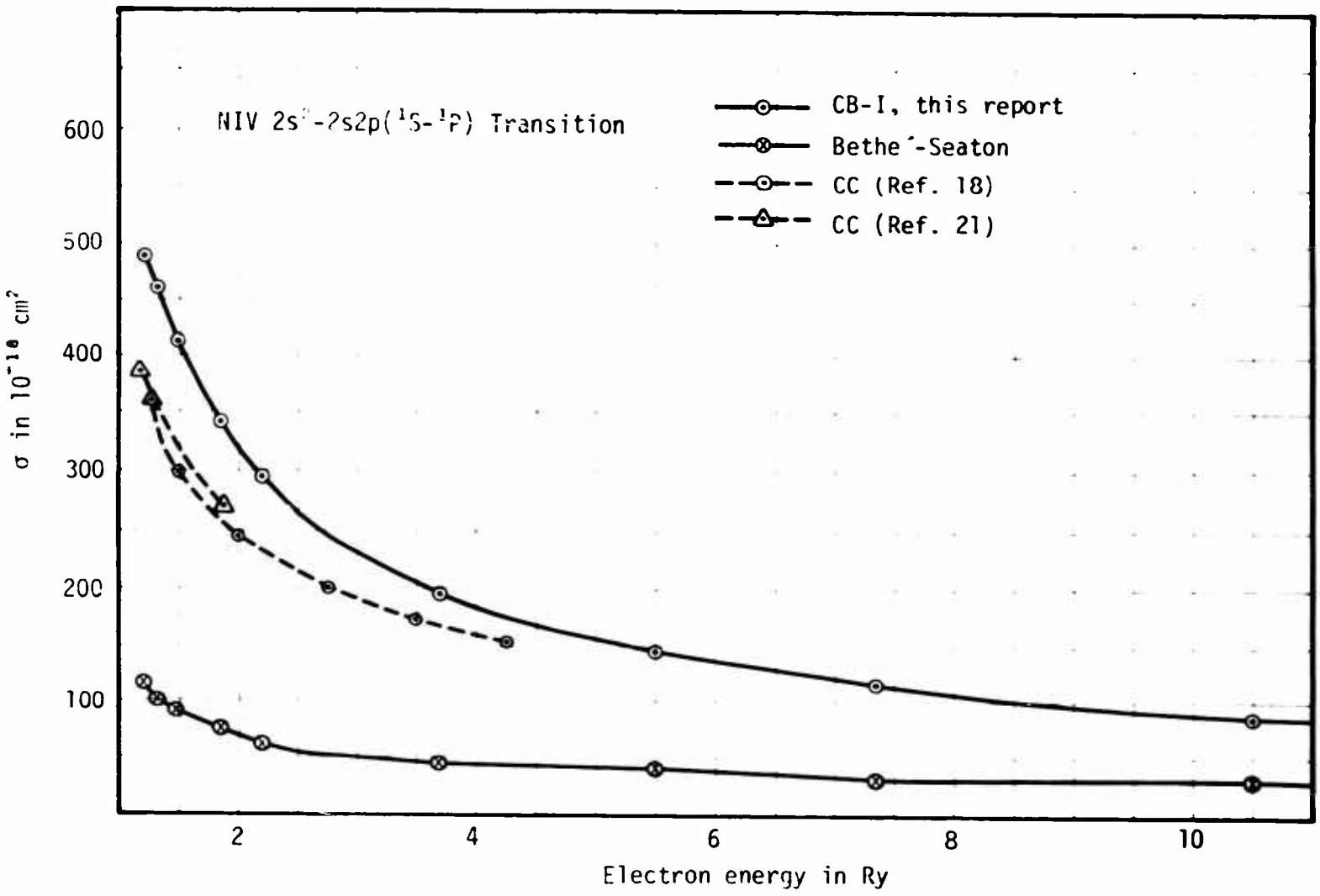

Figure 8. Comparison of theoretical electron impact excitation cross-sections for NIV.

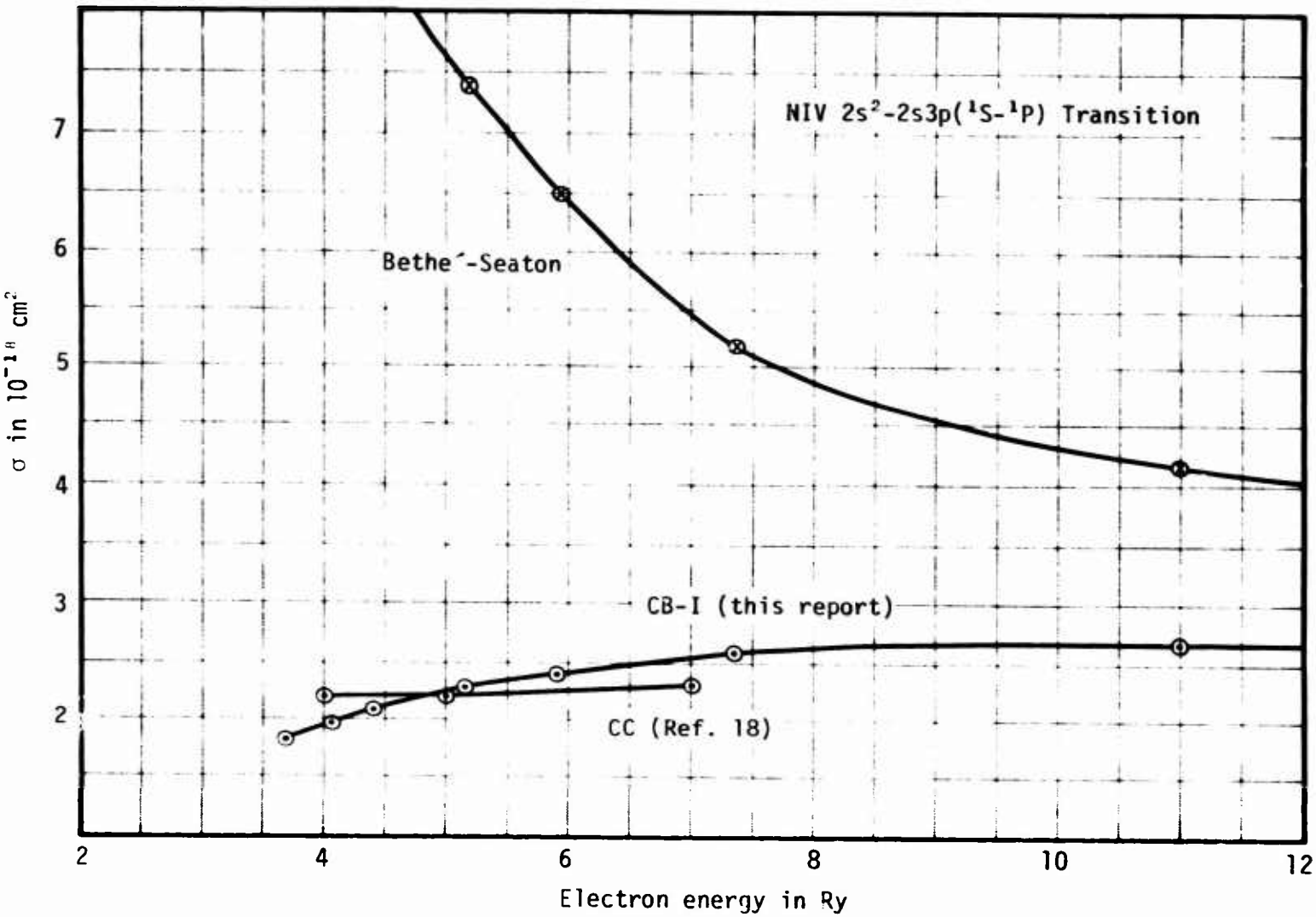

Figure 9. Comparison of theoretical electron impact excitation cross sections for NIV.

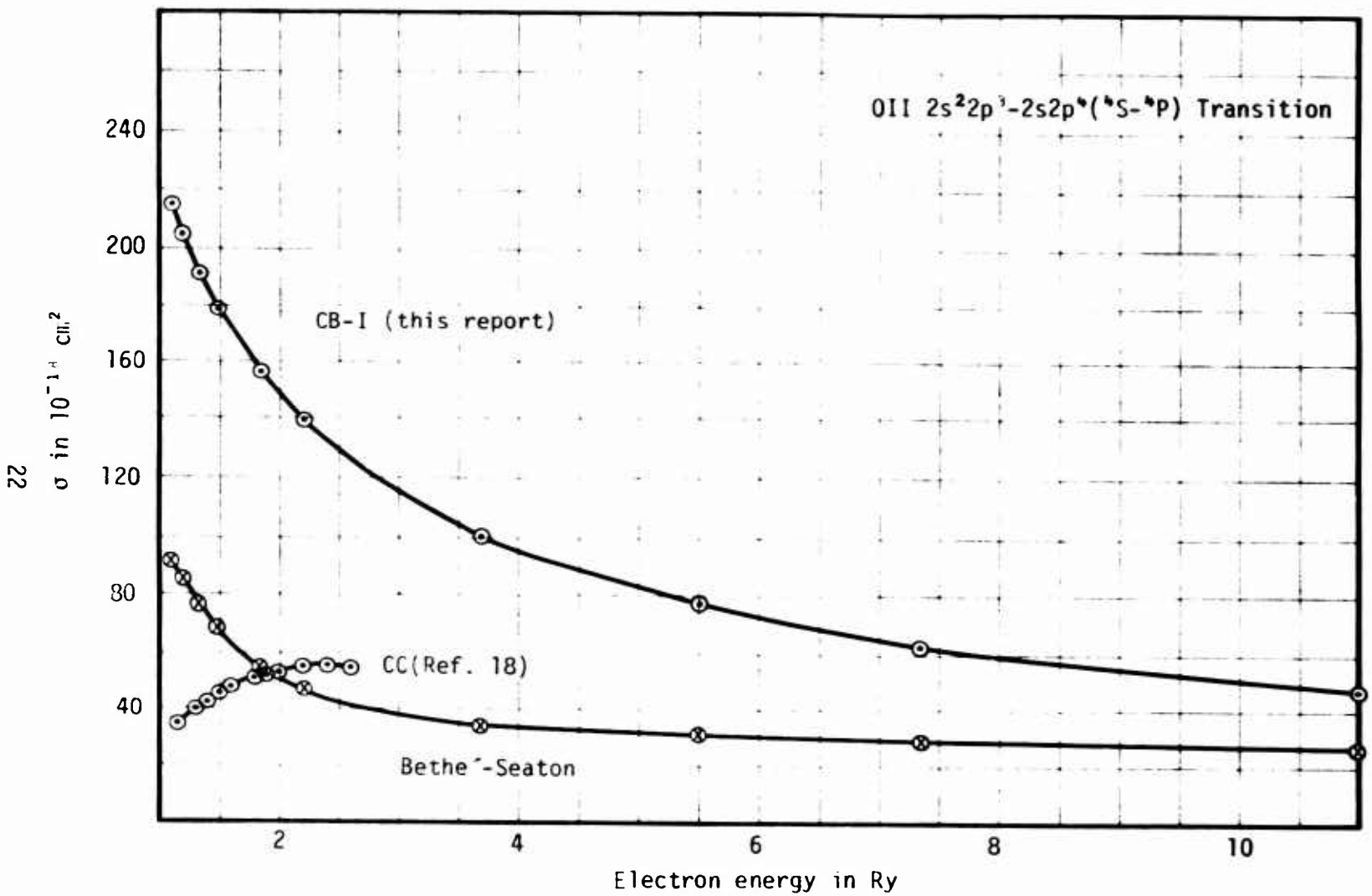

Figure 10. Comparison of theoretical electron impact excitation cross sections for OII.

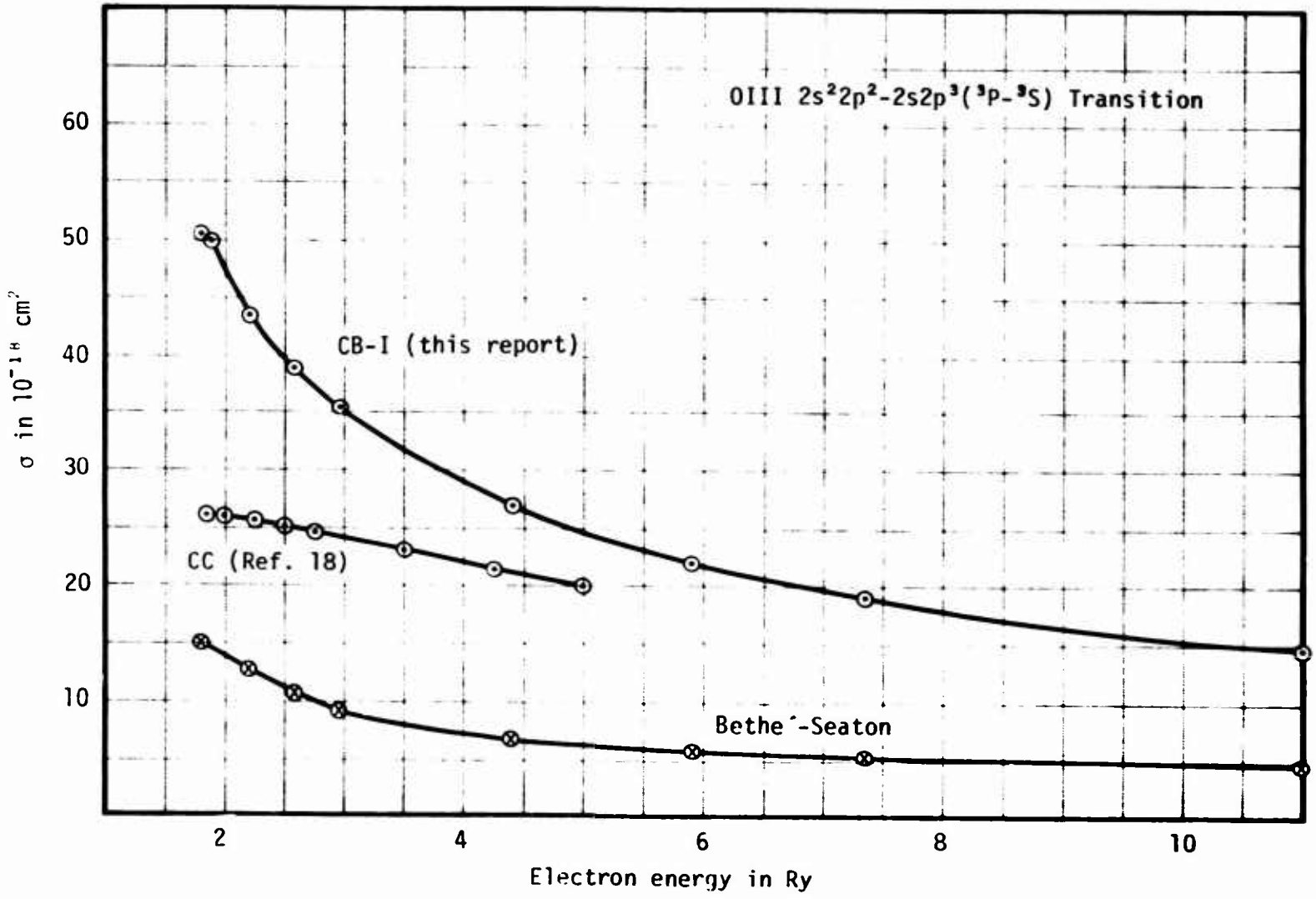

Figure 11. Comparison of theoretical electron impact excitation cross-sections for OIII.

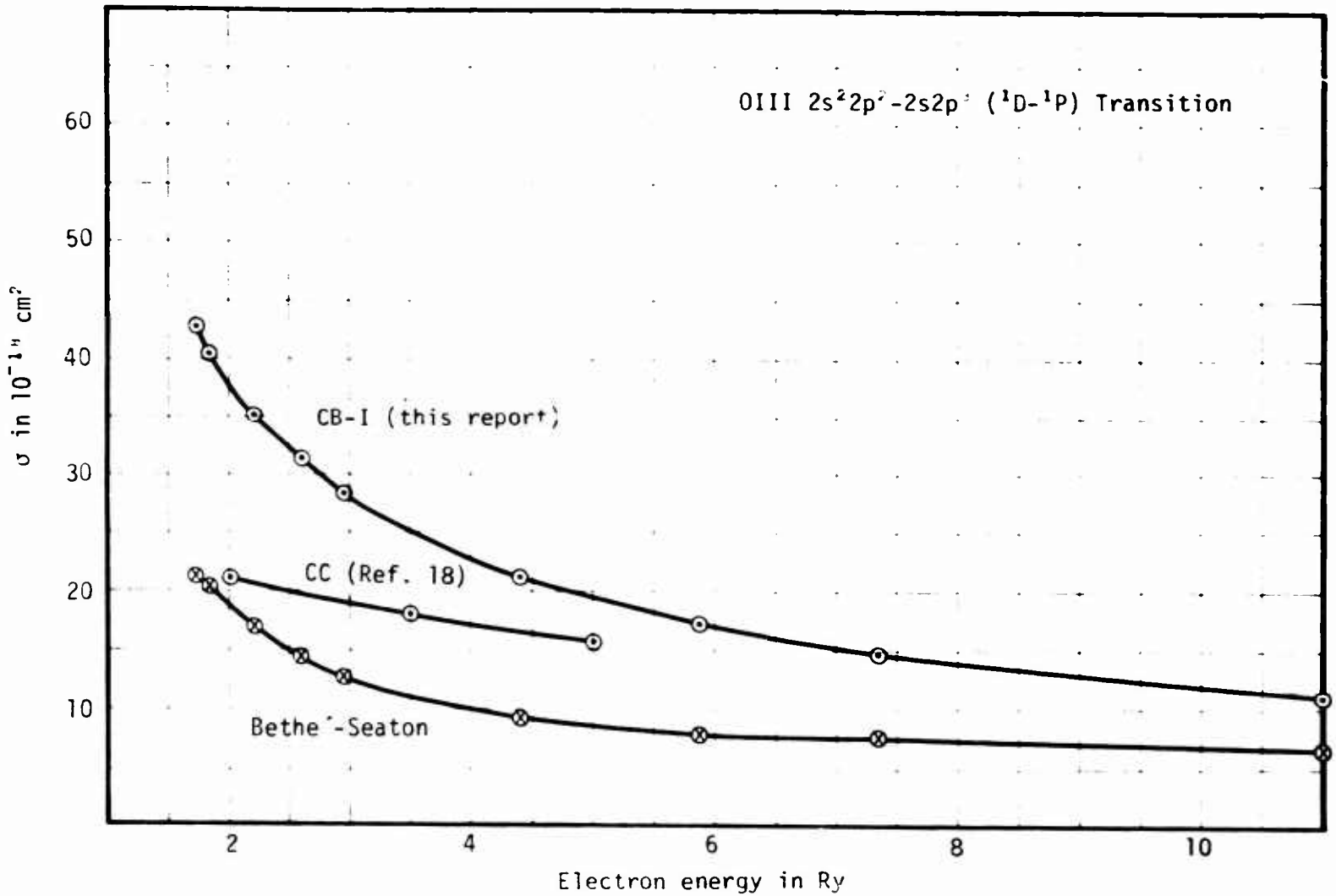

Figure 12. Comparison of theoretical electron impact excitation cross-sections for OIII.

anamolous values in the CC scheme. In contrast, the inter-shell 2s-3p NIV excitation is over-estimated by a considerable amount by the semi-empirical values.

This general trend is exhibited by all thirty CB-I cross-sections calculated here. That is, the intra-shell semi-empirical values are, on the whole, less than the CB-I results and these differences are larger near the threshold where they range from factors of 1.5 to about 4.5. At high energies the discrepancies are less severe and lie in the range of from 1.0 to 3.0. For inter-shell transitions the situation is reversed. The Bethe´-Seaton formula predicts cross-sections that are generally larger than the CB-I values near the threshold (by factors of from 2.9 to 5.6). Again, at higher energies these excitations give better agreement with the two methods differing by factors of around 1.0 to 2.8. The four p-d transitions give the best agreement and never differed by more than 40% throughout the entire incident energy range covered.

The Bethe´-Seaton cross-section is directly proportional to both the oscillator strength, f and the effective Gaunt factor, $\bar{g}$,

$$\sigma = (8\pi/\sqrt{3})(f\,\bar{g}/k_0^2\,\Delta E) \quad , \tag{4}$$

where ΔE is the transition energy. It is derivable from the CB-I approach by assuming that the long-range part of the dipole integral in the R-matrix (see Equation 3) is larger than any other contributions to the collision strength[13]. Allen's $\bar{g}$ values are estimates based on mostly inter-shell type transitions for single electron ions. They apparently are not appropriate for the intra-shell excitations considered here. Equation (4) can be used to calculate an effective Gaunt factor given both σ and f. An internally consistent set of $\bar{g}$ values can be determined by taking the f-values to be those obtained from the same HX radial functions used to compute the CB-I

σ values. The results of such calculations are shown in Figures 13 and 14 for selected transitions of each ion. As is evident, the $\bar{g}$-values fall into two groups – those for intra-shell transitions and those for inter-shell transitions. This behavior is exhibited by all thirty $\bar{g}$-values computed. The results are in good agreement with Davis'[26] theoretically computed $\bar{g}$ values for the resonance transitions of atmospheric ions. The trend towards increasing $\bar{g}$ with increasing charge is also exhibited by Davis' Gaunt factors. Our values are slightly higher throughout and this many reflect differences in oscillator strengths as Davis used the NBS values of Weise, et al.[25] Our computed NIV 2s-3p $\bar{g}$-values, however, are somewhat lower than Davis' predicted values near the threshold. Since the CB-I cross-section agrees well with the CC results, this suggests that the $\bar{g}$ values of Allen or Davis may overestimate the inter-shell s-p or p-s excitation cross-sections in the threshold region. At higher energies the differences are less severe. Allen's $\bar{g}$ values are best for the p-d transitions.

Another point which needs to be considered is the question of what f-values to use in the Bethe´-Seaton formula. The "correct" $\bar{g}$ value is essentially a parameter that gives a "correct" CB-I cross-section. However, as we have seen, the evidence tends to suggest that near the threshold, this method over estimates the cross-section. Accurate f-values are becoming available both theoretically and experimentally. The NBS[25] oscillator strengths for some of the transitions studied here are based on CI wavefunction[27] and they are generally lower than our HX computed f-values or Kelly's[28] Hartree-Fock values. Nussbaumer's[29] CI f-values for the Be I ($2s2p - 2p^2$) iso-electronic series show decreases of from 1.0 to 2.5 with respect to the single configuration results of Weiss[30]. His results are also in better agreement with the most recent experimental data. Smith and Weise[31] have made detailed comparisons of the oscillator strengths obtained from different types of wavefunctions. They found that CI oscillator strength were consistently lower than Hartree-Fock (single configuration) oscillator strengths.

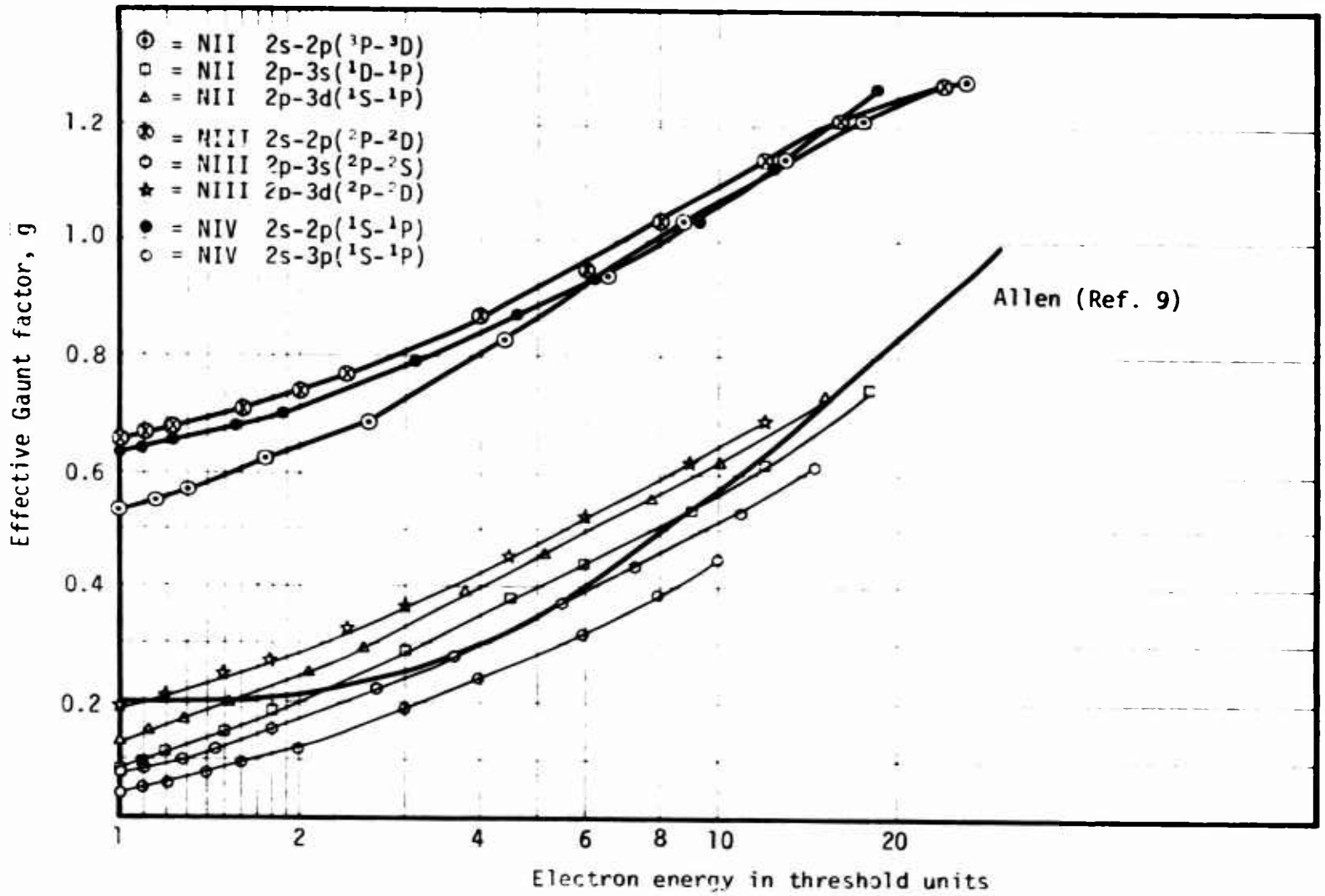

Figure 13. Effective Gaunt factors for selected nitrogen ion transitions.

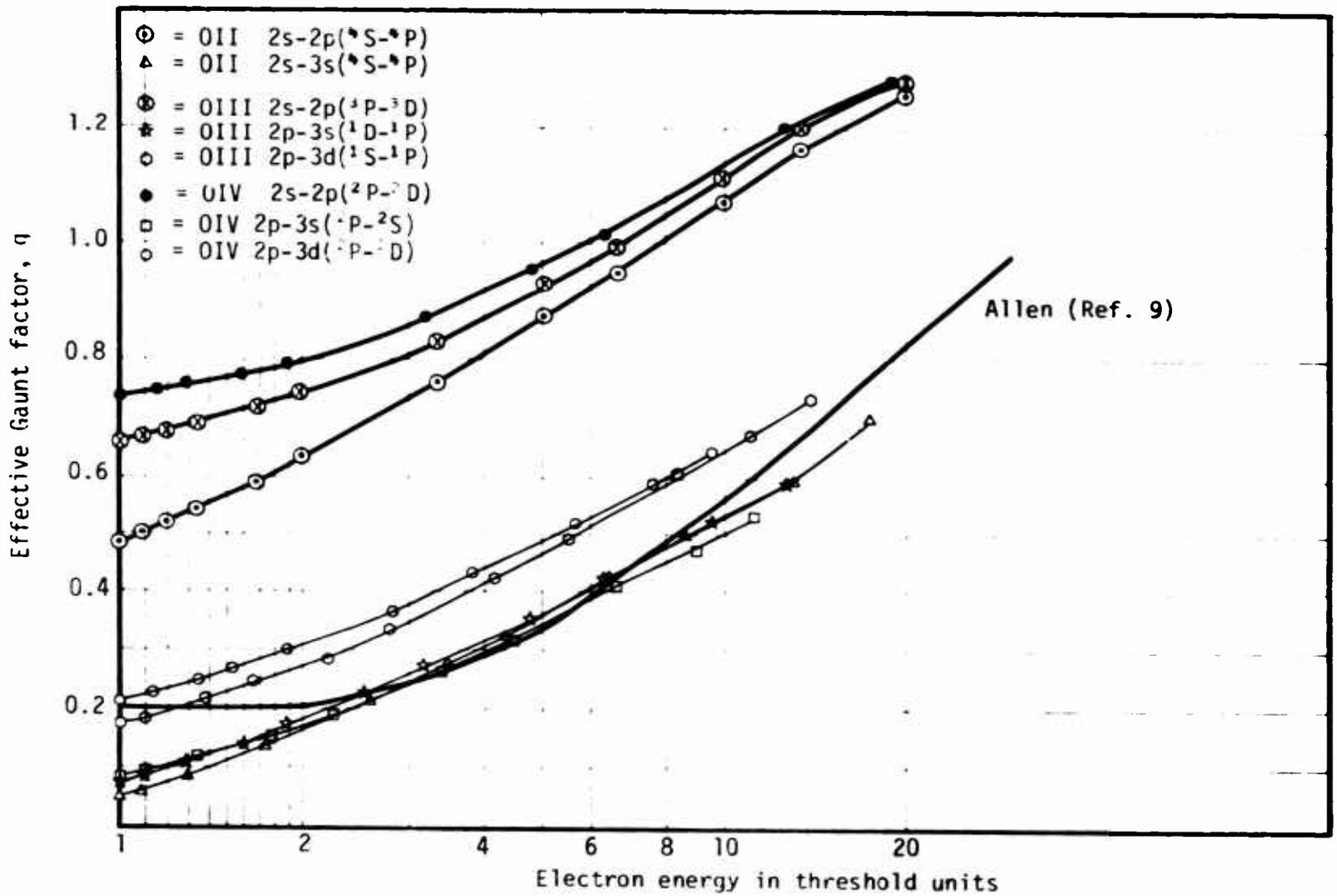

Figure 14. Effective Gaunt factors for selected oxygen ion transitions.

Experimentally determined f-values also tended to be lower than both CI and Hartree-Fock computed values. This suggests that the Bethe'-Seaton formula may be able to give reliable estimates of electron impact excitation cross-sections if accurate f-values are used. It should be kept in mind, however, that the proper $\bar{g}$ values must also be available.

A final point to be made concerning Allen's $\bar{g}$ values for ions is that his values are identical to the $\bar{g}$ values for neutrals for energies of five thresholds or greater. This is probably not realistic and is in disagreement with Tully and Petrini's[12] work on Li-like ions where they found that the Born and Coulomb-Born collision strengths begin to differ by less than 10% only at about eight threshold units.

SECTION 4

SUMMARY AND CONCLUSIONS

Coulomb-Born electron impact excitation cross-sections for thirty transitions from the ground states of the first three ions of nitrogen and oxygen have been computed. The results indicate that the cross-sections can be conveniently classified according to whether the excitation is an intra-shell ($\Delta n = 0$, where n is the principal quantum number) transition or an inter-shell transition ($\Delta n > 0$). The former CB-I cross-sections are generally larger than the latter. Within an iso-electronic series, the CB-I cross-sections decrease with increasing charge. Both of these trends are consistent with other theoretical results.

Based on comparisons with a limited number of more sophisticated calculations[18], the CB-I results tend to over estimate the intra-shell ion cross-sections near the threshold, while for inter-shell transitions the CB-I cross-section may not differ much from the more elaborately calculated values. Factor of two agreement was obtained for all comparisons possible with the exception of the OII reasonance transition.

Cross-sections obtained semi-empirically from the Bethe'-Seaton formula[8] and Allen's $\bar{g}$ values[9] will tend to underestimate the intra-shell transitions and overestimate some of the inter-shell transitions at both low and intermediate energies. Improved $\bar{g}$ values reported here and elsewhere[26] combined with accurate f-values[31] may improve the reliability of this convenient and much used semi-empirical approach.

REFERENCES

1. K. T. Dolder and B. Pearl, J. Phys. B 6, 2415 (1973).
2. P. O. Taylor and G. H. Dunn, Phys. Rev. A 8, 2304 (1973).
3. M. O. Pase and J. W. Hooper, Phys. Rev. A 7, 2033 (1973).
4. I. P. Zapescohnyi, et al., Sov. Phys. JETP 36, 1056 (1973).
5. K. H. Tan, F. G. Donaldson and J. W. McConkey, Can. J. Phys. 52, 786 (1974).
6. D. H. Crandall, et al., Phys. Rev. A 9, 2545 (1974).
7. H. J. Kunze, Space Sci Rev. 13, 565 (1972).
8. M. J. Seaton, in Atomic and Molecular Processes, Ed. D. R. Bates, 374-420, Academic Press, New York (1962).
9. C. W. Allen, Astrophysical Quantities, Athlone Press, London (1973).
10. H. Van Regemorter, Astrophys. J. 136, 906 (1962).
11. J. A. Keefer, "Coulomb-Born Electron Impact Excitation Cross-Section for NII $^3P(2s^22p^2)$-$^3D(2s2p^3)$ Transition", MRC-R-101, Nov. 1973.
12. I. G. Percival and M. J. Seaton, Proc. Camb. Phil. Soc. 53, 654 (1957).
13. H. Van Regemorter, Mon. Not. Roy. Astron. Soc. 121, 213 (1960).
14. F. A. Sharpton, R. M. St. John, C. C. Lin and F. E. Fajen, Phys. Rev. A 2, 1305 (1970).
15. H. Nussbaumer, Computer Phys. Commun. 1, 191 (1969).
16. R. D. Cowan, Phys. Rev. 164, 54 (1957).
17. C. Moore, Atomic Energy Levels, U.S. NBS Circular No. 467 (1949).

18. S. Ormande, K. Smith, B. W. Torres and A. R. Davies, Phys. Rev. A 8, 262 (1973).

19. J. A. Tully, J Phys. B 7, 386 (1974).

20. J. A. Tully, Can. J. Phys. 51, 2047 (1973).

21. D. E. Osterbrook, J. Phys. B 3, 149 (1970).

22. H. E. Seraph and M. J. Seaton, J. Phys. B 7, L36 (1974).

23. B. L. Moiseiwitsch and S. J. Smith, Rev. Mod. Phys. 40, 238 (1968).

24. D. R. Flower, J. Phys. B 4, 697 (1971).

25. W. L. Weise, M. W. Smith and B. M. Glennon, Atomic Transition Probabilities, Vol. I, NSRDS-NBS 4 (1966).

26. J. Davis, J. Quant. Spectrosc. Radiat. Transfer 14, 549 (1974).

27. A. B. Bolotin, I. B. Levinson and L. I. Levin, Sov. Phys. JETP 2 391 (1956).

28. P. S. Kelly, Astrophys. J. 140, 1247 (1964).

29. H. Nussbaumer, Astron. and Astrophys. 16, 77 (1972).

30. A. Weiss, Astrophys. J. 138, 1262 (1963).

31. M. W. Smith and W. L. Weise, Astrophys. J. Suppl. Ser. No. 196, 23, 103 (1971).

32. J. A. Tully and D. Petrini, J. Phys. B 7, L231 (1974).